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Mathematical model for the diffusion of low-molecula--mass substance into polymer material

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Abstract

A mathematical model is proposed to explain the diffusion of a low-molecular-mass substance into polymer particles. This model takes into account the variation of the structure, weight, and volume of particles. The expression for the shrinkage velocity of particles during solvent extraction is derived from the mass-balance equation. This excludes the need to preset this value. The advanced model assumes the existence of a mobile interface. Therefore, a difference scheme is constructed taking into account the transition from a variable to a fixed region. Realization of the difference scheme allows one to determine the solvent concentration profile inside a particle at each moment of time, the shrinkage velocity of a particle, and the kinetic characteristics of the solvent extraction process.